

# 2-Propenoic acid, 3-cyano-, methyl ester, (Z)-

<b>Inchi:</b>	InChI=1S/C5H5NO2/c1-8-5(7)3-2-4-6/h2-3H,1H3/b3-2-
<b>InchiKey:</b>	AJXIQWIGXITQSV-IHWYPQMZSA-N
<b>Formula:</b>	C5H5NO2
<b>SMILES:</b>	COC(=O)C=CC#N
<b>Mol. weight [g/mol]:</b>	111.10
<b>CAS:</b>	925-55-3

## Physical Properties

Property code	Value	Unit	Source
gf	-29.30	kJ/mol	Joback Method
hf	-109.23	kJ/mol	Joback Method
hfus	13.20	kJ/mol	Joback Method
hvap	46.32	kJ/mol	Joback Method
log10ws	-0.50		Crippen Method
logp	0.239		Crippen Method
mcvol	85.830	ml/mol	McGowan Method
pc	3786.98	kPa	Joback Method
tb	496.33	K	Joback Method
tc	706.59	K	Joback Method
tf	278.18	K	Joback Method
vc	0.345	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	164.90	J/molxK	496.33	Joback Method
cpg	171.44	J/molxK	531.37	Joback Method
cpg	177.66	J/molxK	566.42	Joback Method
cpg	183.57	J/molxK	601.46	Joback Method
cpg	189.16	J/molxK	636.51	Joback Method
cpg	194.46	J/molxK	671.55	Joback Method
cpg	199.46	J/molxK	706.59	Joback Method

# Sources

<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C925553&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C925553&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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